Physics-based Preconditioners for Ocean Simulation

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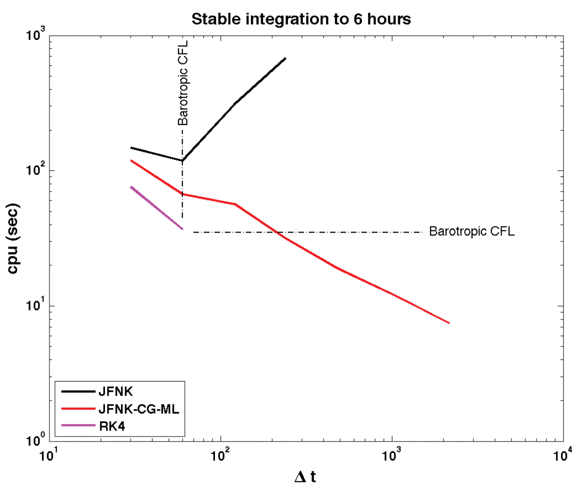
Physics-based preconditioning is a highly successful approach for multiple-time-scale problems where an accurate simulation is desired on the dynamical time scale. In our research we are developing physics-based preconditioners for ocean simulation based on barotropic-baroclinic splitting. Our approach is a fully implicit, fully coupled time integration of the momentum and continuity equations of ocean dynamics, thus reducing the error and increasing the stability of traditional operator splitting. The nonlinear system is solved via preconditioned Jacobian-free Newton-Krylov, where we reformulate traditional barotropic-baroclinic splitting as a preconditioner. Thus the desired solution is time step converged with time steps on the order of the dynamical time scale, a crucial feature as we scale to exascale simulation.

Fig. 1. Timestep size versus CPU time for explicit Runge-Kutta (RK4), unpreconditioned implicit Euler (JFNK) and preconditioned implicit Euler (JFNK-CG-ML). Implicit methods afford a stable integration with much larger time steps than explicit methods; preconditioned implicit Euler utilizes time steps on an order of 30 times the barotropic time scale. However, the key to efficient, scalable implicit methods is effective preconditioning; implicit Euler preconditioned with the barotropic system scales on the same order as Runge-Kutta, while unpreconditioned implicit Euler does not scale beyond the barotropic timescale.



Due to numerical stability issues, low-order accuracy and inherent step-size restrictions associated with traditional explicit, split-explicit, and semi-implicit time integration methods, implicit time integration will be required for high-resolution ocean modeling. We are developing physics-based preconditioners for implicit ocean simulation that allow enhanced accuracy, stability, and the ability to time integrate with time steps much larger than explicit or semi-implicit methods currently in practice. Our implicit time integration is implemented with Jacobian-free Newton-Krylov (JFNK) as a nonlinear solver [1]. The JFNK framework allows tighter coupling of the physics, thus reducing errors and increasing stability inherent to operator splitting. In addition, higher-order implicit time integration schemes are easily implemented in the JFNK framework. The key to effective implementation of JFNK is effective preconditioning. As time-step sizes in explicit and split-explicit methods are dictated by the barotropic time scale, we have implemented a barotropic solver as a physics-based preconditioner, based on implicit time integration of the barotropic system over the baroclinic time interval, which allows efficient implicit time integration on the order of the baroclinic time scale.

Following the standard prescription for physics-based preconditioning, we reformulate the current ocean simulation semi-implicit solver [2] as a preconditioner. The ocean model is decoupled into baroclinic and barotropic systems. The barotropic system is a 2D hyperbolic system (obtained by vertical integration of the full system) that isolates the stiff external gravity wave and can easily be decoupled to a parabolic system for a scalar variable that can be integrated implicitly over the baroclinic time step. This implicit integration necessitates solving a linear system involving an elliptic operator, which can be implemented in a scalable way using multigrid solver technology. As a result, application of the preconditioner is reduced to a scalable elliptic solve for a 2D scalar variable, rather than solution of a full 3D vector system. This approach allows a split-implicit solver (as found in Parallel Ocean Program, POP), to be used as a solver or preconditioner.

The JFNK framework is implemented in a z-level ocean model prototype via an interface to the nonlinear solver package (NOX) in the Trilinos software from SNL [3]. The nonlinear solve at each time step fully utilizes the JFNK framework in Trilinos with generalized minimum residual method (GMRES) as the linear solver. The linear solve required by the parabolic system for the implicit barotropic preconditioner is implemented with the conjugate gradient (CG) solver in Trilinos, which is in turn preconditioned with algebraic multigrid using the multilevel preconditioning package (ML) package in Trilinos. Results to date indicate that a stable, implicit time integration can be performed with step sizes thirty times larger than explicit methods with favorable scalability in terms of CPU time. Figures 1–3 show an example result from a prototype ocean problem.

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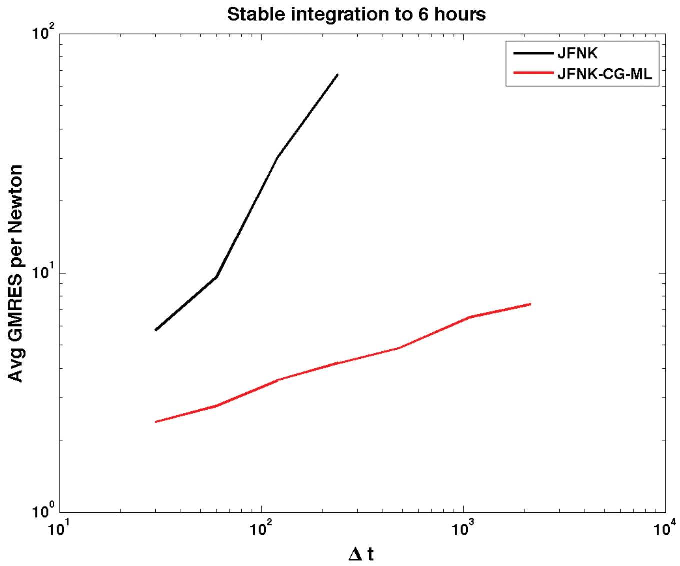

Fig. 2. Time-step size versus average number of GMRES iterations per Newton iteration for unpreconditioned (JFNK) and preconditioned (JFNK-CG-ML) implicit Euler. The dominant cost of JFNK is the number of linear GMRES iterations per Newton iteration. Preconditioning effectively reduces the number of linear GMRES iterations per Newton iteration.

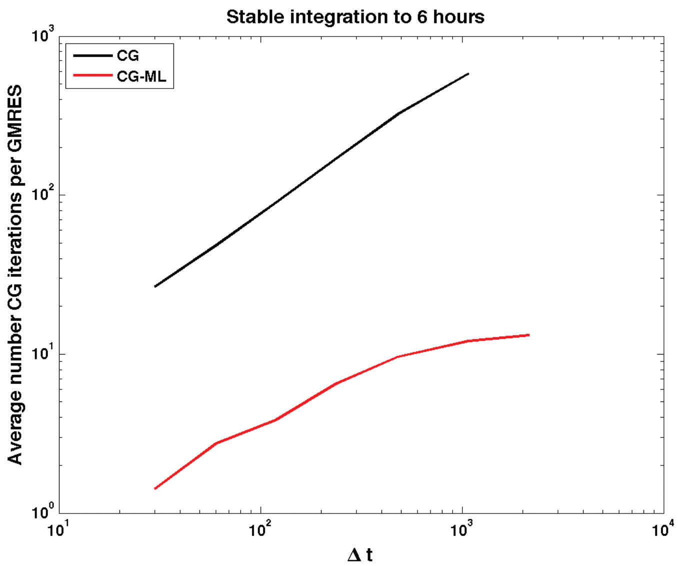

Fig. 3. Time-step size versus average number of CG iterations per GMRES iteration for inversion of the barotropic subsystem without preconditioning (CG) and with multigrid preconditioning (CG-ML). The dominant cost in application of the preconditioner is the number of linear iterations to invert the elliptic operator. Preconditioning of the CG iteration with multigrid methods results in a factor of 10 reduction in CG iterations and exhibits favorable scalability.

We are extending these ideas to co-design efforts in climate science at LANL. As baroclinic-barotropic decoupling is heterogeneous in nature, it readily fits a heterogeneous computing model. The fast-time-scale, 2D barotropic system can be implemented on traditional compute nodes, while the slow time-scale, 3D baroclinic system will be implemented on associated accelerated hardware. This model will allow for a paradigm shift in the use of heterogeneous computing, enabling the effective use of exascale resources. As can be seen, this algorithm shows strong potential in modern high-resolution climate simulations, allowing tighter coupling between the physics, thus reducing errors and increasing stability inherent to operator splitting. Having the ability to perform climate simulations with reduced splitting errors and using variable-resolution grids will be a significant step forward in predictive ocean and sea ice simulation. In addition, there is a clear route to exascale–given the heterogeneous nature of this algorithm, it can be readily mapped to evolving hybrid computing architectures, providing the opportunity for effective co-design.

[1] Knoll, D.A. and D.E. Keyes, *J Comput Phys* **193,** 357 (2004).
[2] Dukowicz, J.K. and R.D. Smith, *J Geophys Res* **99,** 7991 (1994).
[3] Heroux, M. et al., http://trilinos.sandia.gov (2008).

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